Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

An *Ab Initio* Study of SiC Double-Walled Nanotubes of Types 2 and 3[1] KAPIL ADHIKARI, ASOK RAY, Department of Physics, University of Texas at Arlington — A hybrid density functional study of armchair SiC double walled nanotubes (DWNTs) of types 2 and 3 is presented. The geometries of individual DWNTs of types 2 and 3 have been spin optimized using the hybrid functional B3LYP (Becke's three-parameter exchange functional and the Lee-Yang-Parr exchange-correlation functional) and the basis set 3-21G* and the GAUSSIAN 09 software. A study of binding energies, Mulliken charge, density of states and HOMO-LUMO gaps has been performed for all nanotubes from (n,n)@(n+3,n+3) to (n,n)@(n+6, n+6) (n=3-6). Type 2 DWNTs do not conserve the coaxial geometry when the difference in chirality of outer and inner tube is 5 or less. For type 3, this occurs when the chirality difference of 4 or less. The gaps of types 2 and 3 DWNTs are less then the corresponding single-walled nanotubes and are significantly less than those of type 1 DWNTs.

[1]This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525).

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Date submitted: 16 Nov 2010 Electronic form version 1.4